Efficiently Learning the Graph for Semi-supervised Learning

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Introduction

We consider graph-based approaches for semi-supervised learning on large datasets. Known techniques to improve efficiency typically involve an approximation of the graph regularization objective, however:

- The graph is assumed to be known or constructed with heuristic hyperparameter values
- They do not provide a principled approximation guarantee for learning over the full unlabeled dataset.

We propose algorithms that overcome both limitations.

- We learn the graph $G(\sigma)$ via algorithms that can exhaustively search a continuous parameter space
- We give an online learning framework to learn the graph efficiently online
- We speedup our algorithm by using the Conjugate Gradient method as an approximate matrix inversion method
- We give guarantees of our algorithm given approximate feedback
- We observe significant (~10-100x) speedup over prior work

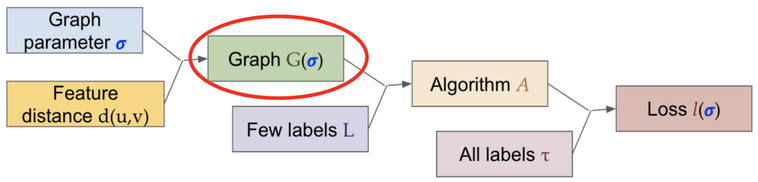


Figure 1. A visual of the semi-supervised learning setup. We learn graph $G(\sigma)$ by finding optimal σ

Online Learning Setup

Dispersion. Consider a parameter space $\mathcal{C}$, a sequence of random loss functions $l_1, \dots, l_T$: $\mathcal{C} \to [0,1]$, and a constant β. We consider this random sequence β-dispersed for Lipschitz constant L if, for all $\epsilon \geq T^{-\beta}$, each pair of points at distance ϵ in $\mathcal{C}$ is not L-Lipschitz for at most $\tilde{O}(\epsilon \mathrm{T})$ functions in expectation.

An online optimization problem with loss functions $l_1, l_2, \dots$ is said to have (ϵ, γ)**-approximate semi-bandit feedback** with system size M if there is a partition $\tilde{A}_t^{(1)}, \dots \tilde{A}_t^{(m)}$ of the parameter space $\mathcal{P} \subset \mathbb{R}^d$, such that if the learner plays point $\rho_t \in \tilde{A}_t^{(i)}$, she observes approximate feedback set $\tilde{A}_t^{(i)}$ and approximate loss $\tilde{l}_t(\rho)$, which is within γ of the loss for all $\rho_t \in \tilde{A}_t^{(i)}$ except for some subset of $\tilde{A}_t^{(i)}$ with volume at most ϵ.

Algorithm 1: Approximate Continuous exp3-set (λ)

Input: step size $\lambda \in [0, 1]$.
Initialize $w_1(\rho) = 1$ for all $\rho \in \mathcal{P}$.
for $t = 1, \dots, T$ **do**
  Sample ρ_t according to $p_t(\rho) = \frac{w_t(\rho)}{\int_{\mathcal{P}} w_t(\rho) d\rho}$.
  Play ρ_t and suffer loss $l_t(\rho_t)$.
  Observe (γ, ϵ)-approximate feedback $\tilde{l}_t(\rho)$ over set $\tilde{A}_t$ with $\rho_t \in \tilde{A}_t$
  Update $w_{t+1}(\rho) = w_t(\rho) \exp(-\lambda \hat{l}_t(\rho))$, where $\hat{l}_t(\rho) = \frac{\mathbf{I}\{\rho \in \tilde{A}_t\}}{\int_{\tilde{A}_t} p_t(\rho) d\rho} \tilde{l}_t(\rho)$.

Online Learning Guarantees

Regret bound for Algorithm 1. Suppose $l_1, \dots, l_T$: $\mathcal{C} \to [0,1]$ is a sequence of loss functions that is β-dispersed, and the domain $\mathcal{C} \subset \mathbb{R}^d$ is contained in a ball of radius R. Algorithm 1 achieves expected regret

$$\tilde{O}\left(\sqrt{dMT \log RT} + T^{1-\min\{\beta,\beta'\}}\right)$$

with access to (ϵ, γ)-approximate semi-bandit feedback with system size M, provided $\gamma \leq \text{volume}\left(\mathfrak{B}\left(T^{-\beta}\right)\right) T^{-\beta}$, where $\mathfrak{B}(r)$ is a d-ball of radius r.

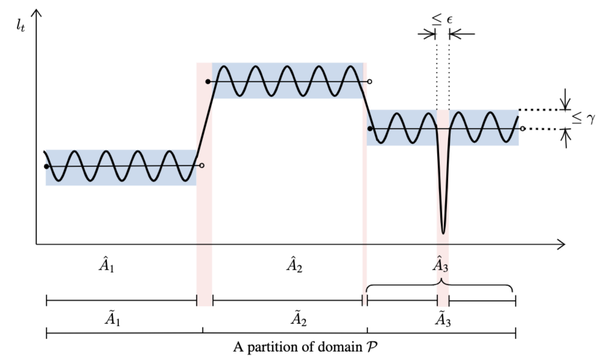


Figure 2. A depiction of a (ϵ, γ)**-approximate semi-bandit feedback** with system size 3.

Graph Learning Setup

Gaussian nearest neighbors. Consider a data space $\mathcal{X}$ and distance function $d: \mathcal{X} \times \mathcal{X} \to \mathbb{R}_{\geq 0}$. Further, let N'_k denote a subset of $\mathcal{X} \times \mathcal{X}$, where $(u, v) \in N'_k$ indicates u is a k-nearest neighbor to v AND v is a k nearest neighbor to u under metric $d(\cdot,\cdot)$. Finally, construct graph $G(k, \sigma)$ with edge weights:

$$w(u, v) = e^{\frac{d(u,v)^2}{\sigma^2}} \mathbb{I}[(u, v) \in N'_k]$$

for all instances $u, v \in \mathcal{X}$. We let $\mathcal{H}_{k,\sigma}$ denote a set of functions that take in some $k \in [K], \sigma \in \mathbb{R}$ and output loss w.r.t. label predictions on graph $G(k, \sigma)$.

Pseudo-dimension of $\mathcal{H}_{k,\sigma}$. We show that the pseudo-dimension of $\mathcal{H}_{k,\sigma}$ is $O(K + \log n)$, where n denotes the number of nodes in the graph, and the labeling algorithm is the mincut approach of Blum and Chawla [2001].

Algorithm 2: Approximate Feedback Set (ϵ, η)

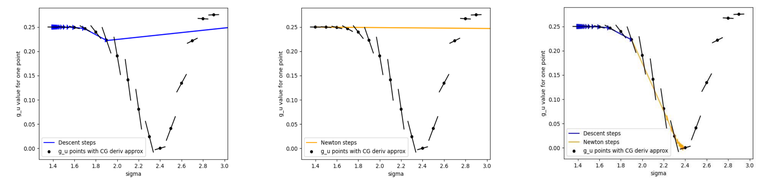
Input: Graph G with unlabeled nodes U, labels f_L, query parameter σ_0, error tolerance ϵ, learning rate η, algorithm $\mathcal{A}$ to estimate soft labels and derivatives at any σ
Output: Estimates for piecewise constant interval containing σ_0, and function value at σ.
for all $u \in U$ **do**
  while $|\sigma_{n+1} - \sigma_n| \geq \epsilon$ **do**
    Compute $f_{u,\epsilon}(\sigma), \frac{\partial f_u}{\partial \sigma}_{\epsilon}$ as $\mathcal{A}(G, f_L, u, \sigma_n, \epsilon)$, where f is the soft label function
    Set $g_u(\sigma_n) = (f_{u,\epsilon}(\sigma_n) - \frac{1}{2})^2$
    Compute Gradient Descent and Newton's method steps $\xi_{\text{GD}}, \xi_{\text{Newton}}$ for $g_u(\sigma_n)$
    Step σ_{n+1} towards σ^*, where $g_u(\sigma^*) = 0$ by setting $\sigma_{n+1} = \sigma_n - \min\{\xi_{\text{GD}}, \xi_{\text{Newton}}\}$.
  $\sigma_l = \min\{\sigma_l, \sigma_{n+1}\}, \sigma_h = \max\{\sigma_h, \sigma_{n+1}\}, n \leftarrow n + 1$.
return $[\sigma_l, \sigma_h]$, $f_\epsilon(\sigma_0)$.

Graph Learning Guarantees

Complexity bound for Algorithm 2. Given an algorithm for computing ϵ-approximate soft labels and gradients for the efficient semi-supervised learning algorithm of Delalleau et al. [2005], Algorithm 2 computes (ϵ, ϵ)-approximate semi-bandit feedback for loss $l(\sigma)$ in time

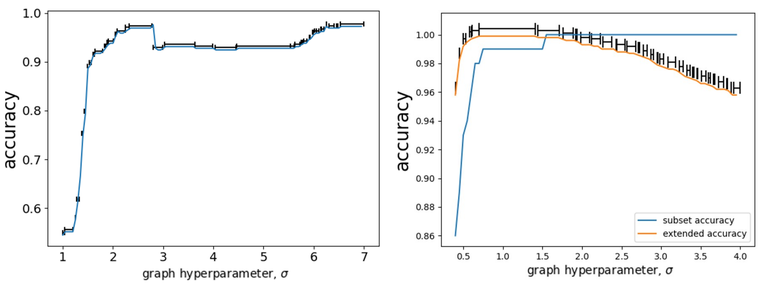
$$O\left(\left|E_{G_{\widetilde{U}}}\right| n\sqrt{\kappa(\mathcal{L}_A)} \log\left(\frac{\lambda\left((|L| + |\widetilde{U}|)\Delta\right)}{\epsilon \sigma_{min} \lambda_{min}(\mathcal{L}_A)}\right) \log\log\frac{1}{\epsilon}\right)$$

Here $E_{G_{\widetilde{U}}}$ represents edges w.r.t. graph of a small subset of unlabeled nodes $\widetilde{U}$, $\mathcal{L}_A$ represents grounded graph Laplacian of graph A used to determine labels for $\widetilde{U}$, and Δ represents the size of the interval for parameter σ. Notice that this bound is linear w.r.t. n, assuming a well conditioned graph.



(a) Gradient Descent Only (b) Newton's Method Only (c) Our Method

Figure 3. An instance where finding local minima of $g_u(\sigma) = \left(f_u(\sigma) - \frac{1}{2}\right)^2$ is challenging. Our method (taking the min of Gradient Descent/Newton's method steps) finds the minima.



(a) Subset of FashionMNIST k=6, 30 |L|=30, |U|=300

(b) Subset of USPS k=6, |L|=10, $|\widetilde{U}|$=100, |U|=1000

Figure 4. Loss intervals calculated with approximate. Black intervals are estimated constant loss.

Results/Discussion

- We show a formal separation in the learning-theoretic complexity of sparse and dense graph families.
- We show how to approximately learn the best graphs from the sparse families efficiently using the conjugate gradient method.
- We provide an online learning framework that can be used to learn the graph efficiently online with sub-linear regret, under mild smoothness assumptions
- We implement our approach and demonstrate significant (~10-100x) speedups over prior work.

References

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